Deep Equilibrium Models

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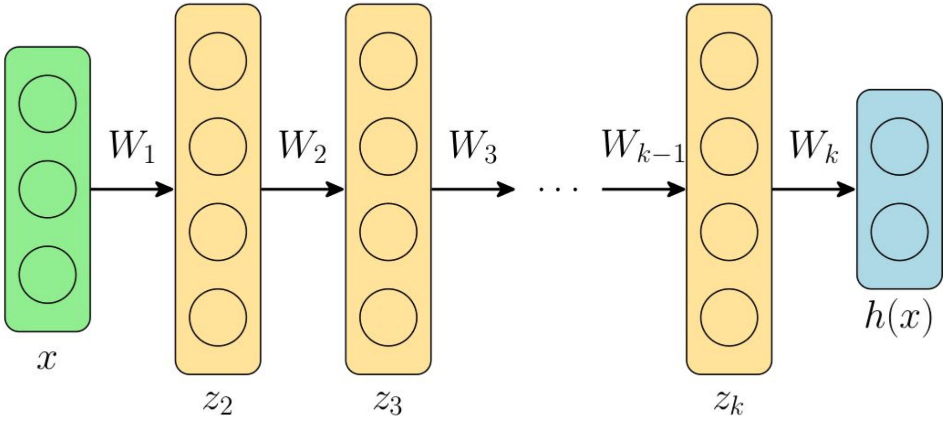
Agenda

1. Weight tying and infinite depth models
2. Implicit layer formulation
3. Approximation and computational considerations
4. DEQ stacking?
5. Experiments

Motivation

Let's start with a typical deep NN architecture:

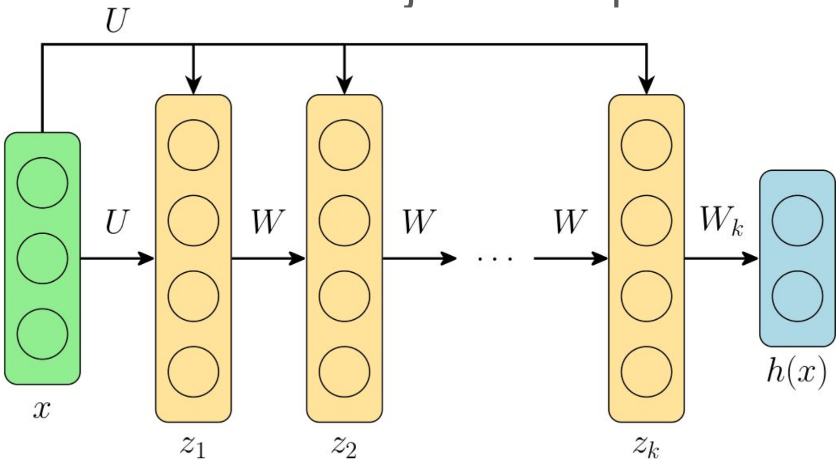


$$
\begin{aligned}
z_1 &= x \\
z_{i+1} &= \sigma(W_i z_i + b_i), \; i = 1, \dots, k-1 \\
h(x) &= W_k z_k + b_k
\end{aligned}
$$

Image courtesy of Deep Implicit Layers Tutorial

Motivation

Weight-Tying: Use the same W and inject the input for each layer



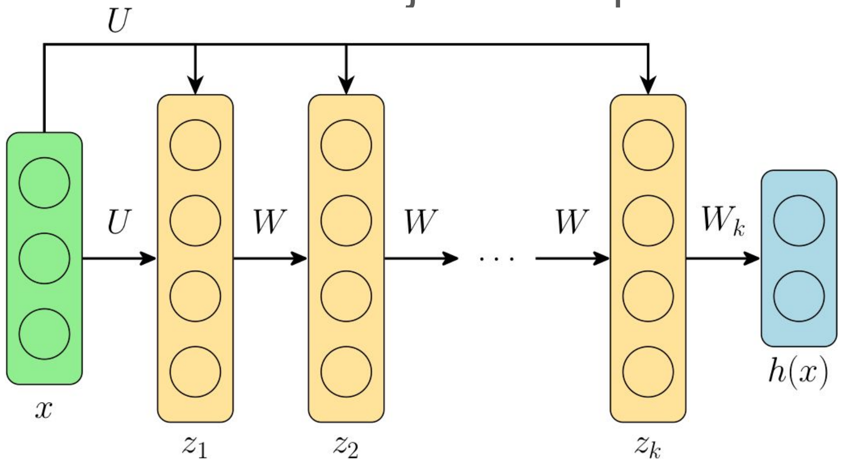
Just as expressive!

$$
\begin{aligned}
z_1 &= 0 \\
z_{i+1} &= \sigma(\boxed{W} z_i + \boxed{U} x + b), \;\; i = 1, \ldots, k-1 \\
h(x) &= W_k z_k + b_k
\end{aligned}
$$

Image courtesy of [Deep Implicit Layers Tutorial]

Motivation

Weight-Tying: Use the same W and inject the input for each layer



Focusing on activation iteration:

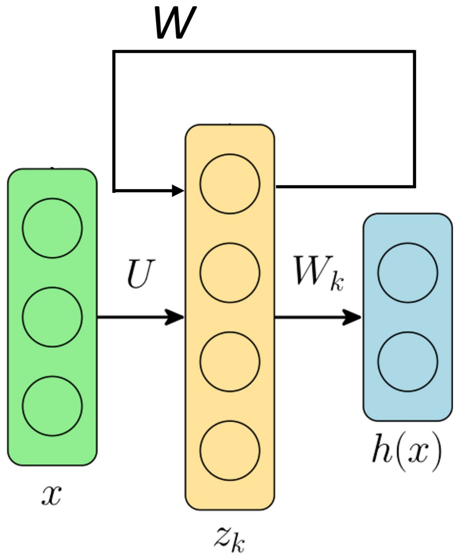
$$z_{i+1} = \sigma(Wz_i + Ux + b), \; i = 1, \ldots, k-1$$

Image courtesy of [Deep Implicit Layers Tutorial]

In the infinite limit, as i -> ∞ (under nice conditions)

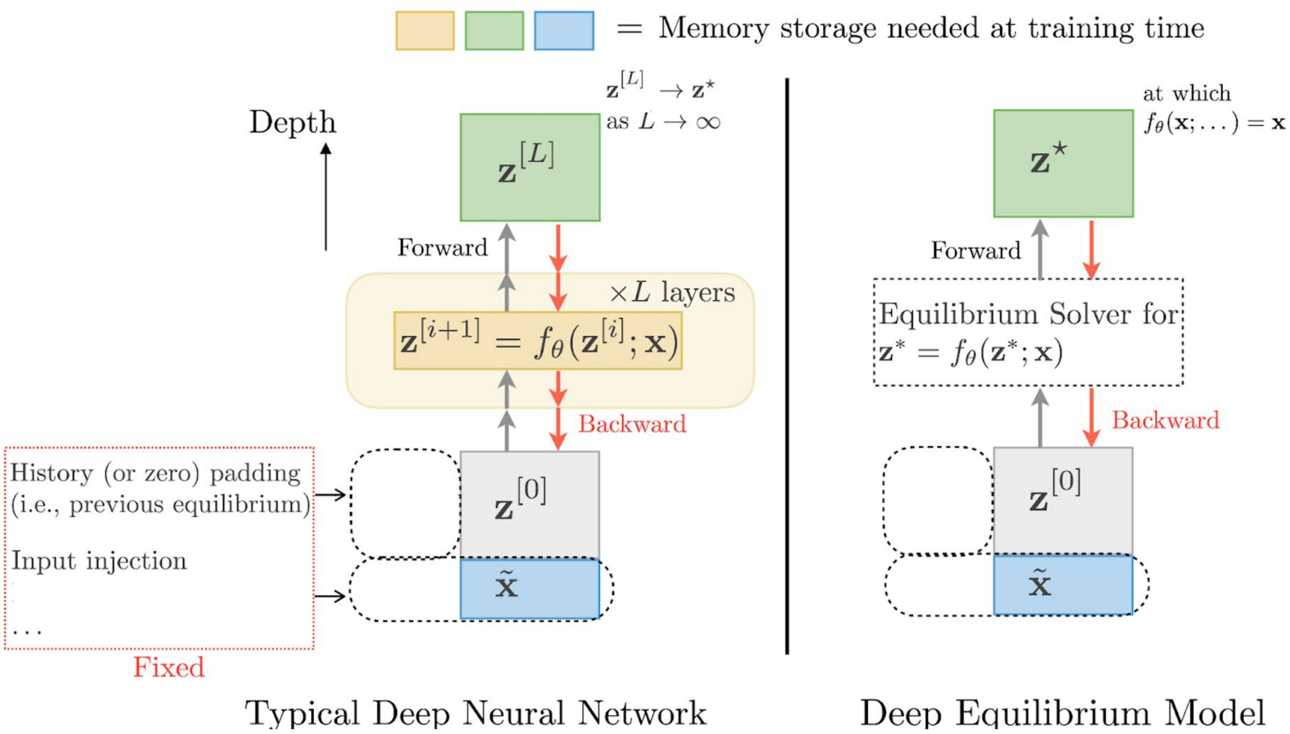
Key insight: The network's activations z* approach a fixed point!

This is a DEQ!



$$\boxed{z^*} = \sigma(W\boxed{z^*} + Ux + b), i \to \infty$$

Deep Equilibrium Model Overview



Implicit vs. Explicit Layers

Explicit Layers:
Typical Neural Network layers, which can directly compute the output and backward pass through backprop

Implicit Layers:
Based on solving solution to some problem, such that **x, z** satisfy some condition

- Arises in naturally in some domains, such as ODEs and *fixed-points*

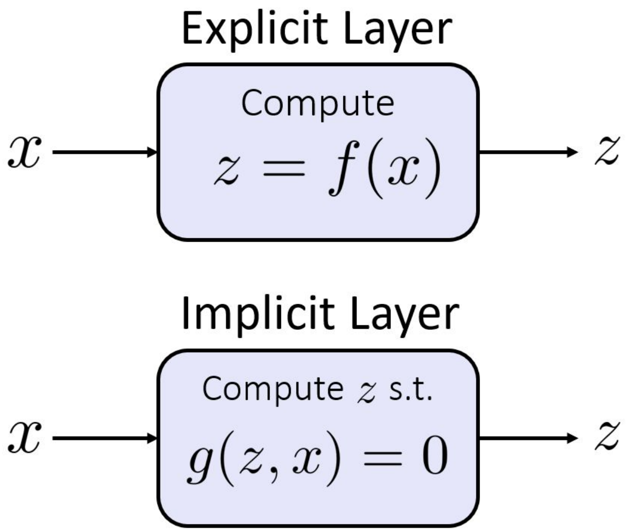


Image courtesy of Deep Implicit Layers Tutorial

Forward Pass

Naive Approach: we could repeatedly apply the function until convergence

$$z^{[i+1]} = f_\theta(z^{[i]}, x) \quad \text{for } i = 0, 1, 2, ...$$

Better Way: Use a root-finding algorithm to find the fixed point

1. Reformulate fixed-point as finding the root:

$$g_\theta(z^*, x) = f_\theta(z^*, x) - z^* \to 0$$

We'll use this notation from here on!

2. Apply generic root-finding algorithm (ex. Newton's method!)

$$\mathrm{z}^* = \mathrm{RootFind}(g_\theta; x)$$

Backward Pass

We need to update the parameters Ɵ in our model, to minimize our loss function

Challenge: differentiating through fixed point $\frac{\partial z^*}{\partial(\cdot)}$

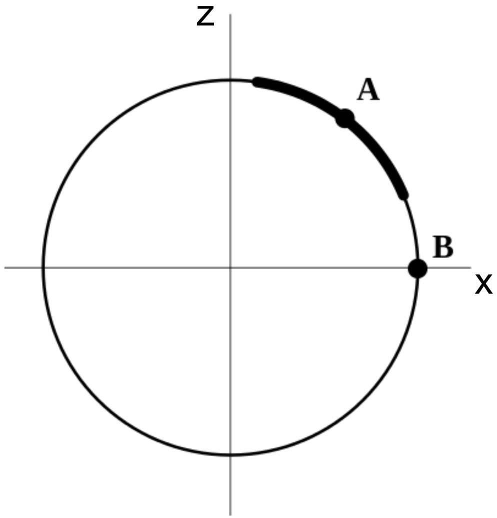
Naive Approach: Built-in Autodiff, through solver computation graph

- Memory Issues
- Floating Point Errors

Better Approach: Use Implicit Function Theorem!

Implicit Function Theorem (Informal)

$$f(x, z) = x^2 + z^2 - 1 = 0$$



Let f be a relation with inputs x_0, z_0

1. $f(x_0, z_0) = 0$
2. f is continuously differentiable with non-singular Jacobian

$$\partial_1 f(x_0, z_0) \in \mathbb{R}^{n \times n}$$

Then there exist neighborhoods (open sets) S_{x_0}, S_{z_0} around x_0 & z_0 and a function $z^* : S_{x_0} \to S_{z_0}$

1. $z_0 = z^*(x_0)$
2. $f(x, z^*(x)) = 0 \quad \forall x \in S_{x_0}$
3. z^* is differentiable on S_{x_0}

Image courtesy of Wikipedia

Implicit Function Theorem

High-level Idea:

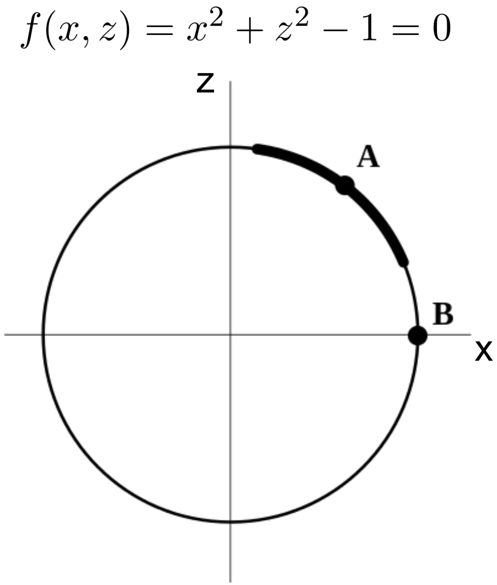
- Convert a relation to a function in a local region and find its derivative

$$f(x, z) = x^2 + z^2 - 1 = 0$$

- Explicit function at A:

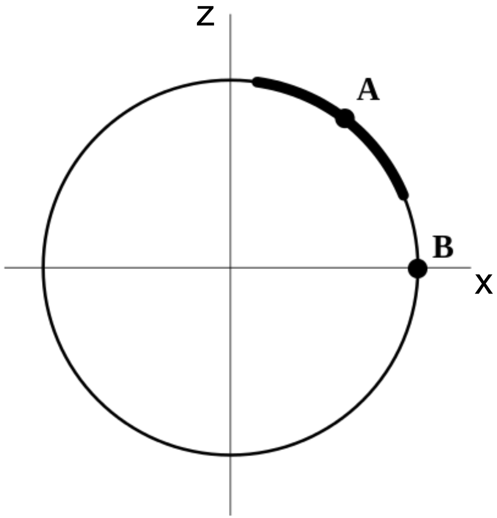
$$g_A(x) = \sqrt{1 - x^2}$$

- IFT allows us to find the derivative of *g*, *without* the explicit form



Implicit Function Theorem

$$f(x,z) = x^2 + z^2 - 1 = 0$$



Let $f : \mathbb{R}^p \times \mathbb{R}^n \to \mathbb{R}^n$ and $x_0 \in \mathbb{R}^p, z_0 \in \mathbb{R}^n$ be such that:

1. $f(x_0, z_0) = 0$
2. f is continuously differentiable with non-singular Jacobian $\partial_1 f(x_0, z_0) \in \mathbb{R}^{n \times n}$

Then there exist open sets $S_{x_0} \subset \mathbb{R}^p$ and $S_{z_0} \subset R^n$ Containing x_0 and z_0 respectively, and a unique continuous function $z^* : S_{x_0} \to S_{z_0}$ such that

1. $z_0 = z^*(x_0)$
2. $f(x, z^*(x)) = 0 \quad \forall x \in S_{x_0}$
3. z^* is differentiable on S_{x_0}

Backwards Pass

$$z_0 = f(x_0, z_0)$$

$$\Big\Downarrow \quad \text{By IFT}$$

$$z^*(x) = f(x, z^*(x)) \quad \forall x \in S_{x_0}$$

$$\boxed{\partial z^*(x_0)} = \partial_0 f(x_0, z_0) + \partial_1 f(x_0, z_0) \boxed{\partial z^*(x_0)}$$

$$\boxed{\partial z^*(x_0)} = [I - \partial_1 f(x_0, z_0)]^{-1} \partial_0 f(x_0, z_0).$$

Backwards Pass - DEQ

- **Backward Pass:**
  - Solve using root finding (e.g. Newtons)

$$\frac{\partial \ell}{\partial (\cdot)} = -\frac{\partial \ell}{\partial z^*}(J_{g_\theta}^{-1}|_{z^*})\frac{\partial f_\theta(z^*;x)}{\partial (\cdot)}$$

$$(J_{g_\theta}^\top|_{z^*})x^\top + (\frac{\partial \ell}{\partial z^*})^\top = 0$$

VJP easily obtained from Pytorch/Jax/etc.

$$g_\theta(z^*;x) = f_\theta(z^*;x) - z^*$$

Approximate Inverse Jacobian - Broyden's Method

- Expensive to calculate the inverse Jacobian during root finding for both forwards and backwards!

- **Broyden's Method (quasi-newton solver):**
    - During root finding, approximates the inverse Jacobian using

$$J_{g_\theta}^{-1}|_{z^{[i+1]}} \approx B_{g_\theta}^{[i+1]} = B_{g_\theta}^{[i]} + \frac{\Delta z^{[i+1]} - B_{g_\theta}^{[i]} \Delta g_\theta^{[i+1]}}{\Delta z^{[i+1]\top} B_{g_\theta}^{[i]} \Delta g_\theta^{[i+1]}} \Delta z^{[i+1]\top} B_{g_\theta}^{[i]}$$

Initial Guess: $B_{g_\theta}^{[0]} = -I$

$$g_\theta(z^*; x) = f_\theta(z^*; x) - z^*$$

DEQ Memory

- **Very memory efficient** because forward and backward passes just use root-finding algorithms.
- Avoids over all the overhead from uncurling backpropagating steps.
- Storage:
  - Equilibrium Point z^*
  - Network Input x
  - Model f_θ
  - VJP (*no Jacobian construction needed!)

Expressivity of DEQs

Intuition:

Consider a simple function composition $$y = g_2(g_1(x))$$
Transforming this into a DEQ:

$$f(z, x) = f\left(\begin{bmatrix} z_1 \\ z_2 \end{bmatrix}, x\right) = \begin{bmatrix} g_1(x) \\ g_2(z_1) \end{bmatrix}$$

Thus, the equilibrium point is:

$$z^\star = f(z^\star, x) \iff z_1^\star = g_1(x),\ z_2^\star = g_2(z_1^\star) = g_2(g_1(x))$$

The output equilibrium is the output of the function!
(can be extended to arbitrary computation graph)

DEQ Stacking?

- Stacking DEQs don't really work, as a single DEQ layer can model any amount of stacked DEQ layers.

Intuition:

Consider a stack of 2 DEQ layers:

$$z_1^\star = f_1(z_1^\star, x) \longrightarrow z_2^\star = f(z_2^\star, z_1^\star)$$

This is equivalent to the following single equilibrium problem:

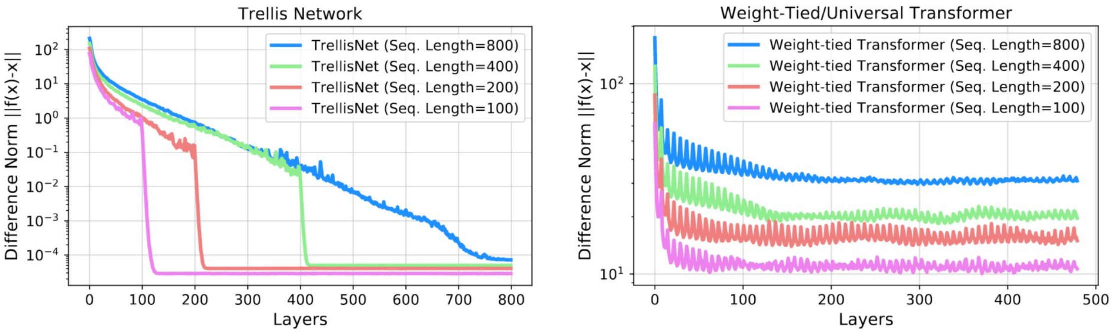
$$z^\star = \begin{bmatrix} z_1^\star \\ z_2^\star \end{bmatrix} = \begin{bmatrix} f_1(z^\star, x) \\ f_2(z_2^\star, z_1^\star) \end{bmatrix} = f(z^\star, x)$$

Experiments

- Apply Deep Equilibrium Networks to sequence modelling tasks
    - Sequence empirically converge
    - Already use of weight tying over the temporal sequence (Trellis Nets & Transformer models)
    - Long-range copy-memory, Penn Treebank Language Modelling, WikiText-103
- Demonstrate the memory efficiency and expressivity of DEQ models given similar parameter counts as well as the speed of computation

Convergence Caveat

- One might expect the network to diverge in the infinite limit
- In practice, many networks do not, which is explored more formally in a later work [Kolter et. al 2020]
- In this work, the authors empirically show that the contributions of subsequent layers diminish at very large depths



Experiments

Word-level Language Modeling w/ WikiText-103 (WT103)				
Model	# Params	Non-Embedding Model Size	Test perplexity	Memory†
Generic TCN [7]	150M	34M	45.2	-
Gated Linear ConvNet [17]	230M	-	37.2	-
AWD-QRNN [33]	159M	51M	33.0	7.1GB
Relational Memory Core [40]	195M	60M	31.6	-
Transformer-XL (X-large, adaptive embed., on TPU) [16]	257M	224M	**18.7**	12.0GB
70-layer TrellisNet (+ auxiliary loss, etc.) [8]	180M	45M	29.2	24.7GB
70-layer TrellisNet with *gradient checkpointing*	180M	45M	29.2	5.2GB
DEQ-TrellisNet (ours)	180M	45M	**29.0**	**3.3GB**
Transformer-XL (medium, 16 layers)	165M	44M	24.3	8.5GB
DEQ-Transformer (medium, ours).	172M	43M	24.2	**2.7GB**
Transformer-XL (medium, 18 layers, adaptive embed.)	110M	72M	23.6	9.0GB
DEQ-Transformer (medium, adaptive embed., ours)	110M	70M	**23.2**	3.7GB
Transformer-XL (small, 4 layers)	139M	4.9M	35.8	4.8GB
Transformer-XL (small, weight-tied 16 layers)	138M	4.5M	34.9	6.8GB
DEQ-Transformer (small, ours).	138M	4.5M	**32.4**	**1.1GB**

Not SOTA, but good at same param size

Efficient!

Experiments - Runtime

Table 4: Runtime ratios between DEQs and corresponding deep networks at training and inference ($> 1\times$ implies DEQ is slower). The ratios are benchmarked on WikiText-103.

DEQ / 18-layer Transformer		DEQ / 70-layer TrellisNet	
Training	Inference	Training	Inference
$2.82\times$	$1.76\times$	$2.40\times$	$1.64\times$

- Notice DEQs are slower!
- This is a consequence of solving an inner optimization inside the network

Conclusion

- Deep Equilibrium Models are a weight tied, approximately infinite depth neural network
  - Output is the fixed point of some neural network function
- Computes two root finding solutions for both the forward and backwards pass
  - Uses IFT to compute the gradient updates rather than backpropagation and autodiff through the iterative graph
- Performs comparatively to SOTA models of the same size but are considerably more memory efficient
  - Typically slower due to the inner loop optimization both forward and backwards

References

Deep Implicit Layers Tutorial - http://implicit-layers-tutorial.org/

Deep Equilibrium Models [Bai 2019] - https://arxiv.org/abs/1909.01377